Large-scale Molecular Dynamics Simulation of Charged Particle Energy Deposition in Strongly Coupled Plasmas

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A promising scheme for producing thermonuclear energy in the laboratory uses charged particle beams to heat hydrogen fuel to very high temperatures. This scheme, known as fast ignition, may employ fast ions, rather than electrons, to heat the fuel—so having a very accurate knowledge of the interaction of fast ions with dense hydrogen fuel is essential. Here we simulate charged-particle stopping in a strongly coupled electron gas using non-equilibrium molecular dynamics. To avoid the challenge of simulating non-equilibrium quantum systems, we initially consider a fictitious system containing classical particles in which the charge of the projectile and the target are the same. Our results can therefore be compared directly to kinetic theory predictions without ambiguity. In the future we will extend our simulations to electron-nucleus mixtures, which will allow us to predict the proportion of energy that goes directly (i.e., instantly) to the ionic fuel without first heating the electrons.

The energy loss per unit length into the fuel, or "stopping power" dE/dx, quantifies the energy deposition from a fast charged particle. This parameter and the related energy split between ions and electrons are important in fast ignition fusion physics [1]. Although there are standard kinetic theory predictions for these quantities, they are mostly limited to describing hot and dilute plasmas. The behavior in cooler, denser plasmas, including the effects of collective excitations, highly-charged impurities, or projectiles, is less certain. Classical molecular dynamics is ideal to study these more relevant scenarios. Modern computational algorithms and architectures permit charged particle simulations with 10^6 to 10^9 particles, usually treating the long-range forces in a particle-particle particle-mesh (PPPM) scheme. Periodic boundary conditions are imposed to mimic the bulk fuel.

We have applied the scalable parallel molecular dynamics (MD) code ddcMD [2] to examine in detail the manner in which fast ions transfer energy to a dense fuel. Here, we consider only the electron component of the fuel, at some temperature T, since that is expected to be the dominant mode of energy loss at relevant projectile energies. We examine energy loss behavior for three different projectile velocities, near the maximum in dE/dx, at velocities ($v \sim 3\, v_{th}$) below the peak, and at high velocities ($v \sim 28\, v_{th}$) above the peak. (We measure the projectile velocity in terms of the mean [thermal] velocity of the electrons in the fuel target, denoted v_{th}.) The simulations described here correspond to a Z=-2 (anti)helium projectile traveling in a low temperature, strongly coupled electron gas with dimensionless Coulomb coupling parameter of order $\Gamma = e^2/(a\, k_B T) = 10$. (This parameter measures the ratio of a typical potential energy e^2/a to a typical kinetic energy $k_B T$; large values correspond to a liquid-like structure.) Like charges are used to prevent bound states, which are unphysically deep, from forming on the projectile. As our comparisons with kinetic theories can easily accommodate this scenario, we lose nothing with this trick.

Our simulations are performed in cubic cells with $N = 128{,}000$ particles. An important issue is that the projectile excites a wake potential, much like the wake behind a boat. Because our system is periodic, our projectile would ride (incorrectly) in the wake of its periodic neighbor. To account for such finite-size effects, we direct the projectile at an oblique angle, to maximize the distance traveled before the projectile's path overlaps the wake from a neighboring replica image. The fastest projectile we consider has $v \sim 28$ Å/fs, so it traverses the cell multiple times during the simulation. This will be further mitigated in the future by using larger simulation cells, and we have recently begun simulations more than an order of magnitude larger than those shown here. For example, these size effects have been explicitly compared (for different conditions than this), and dE/dx is consistent for systems from 6×10^4 to 2×10^6 particles. Our MD simulations provide complete information on the charge-density and current-density perturbations around the moving charged projectile. These perturbations are related to the dielectric response of the target, which may be nonlinear for highly charged projectiles. This dynamical, non-linear response is very difficult to include in standard kinetic theories of charged-particle energy loss.

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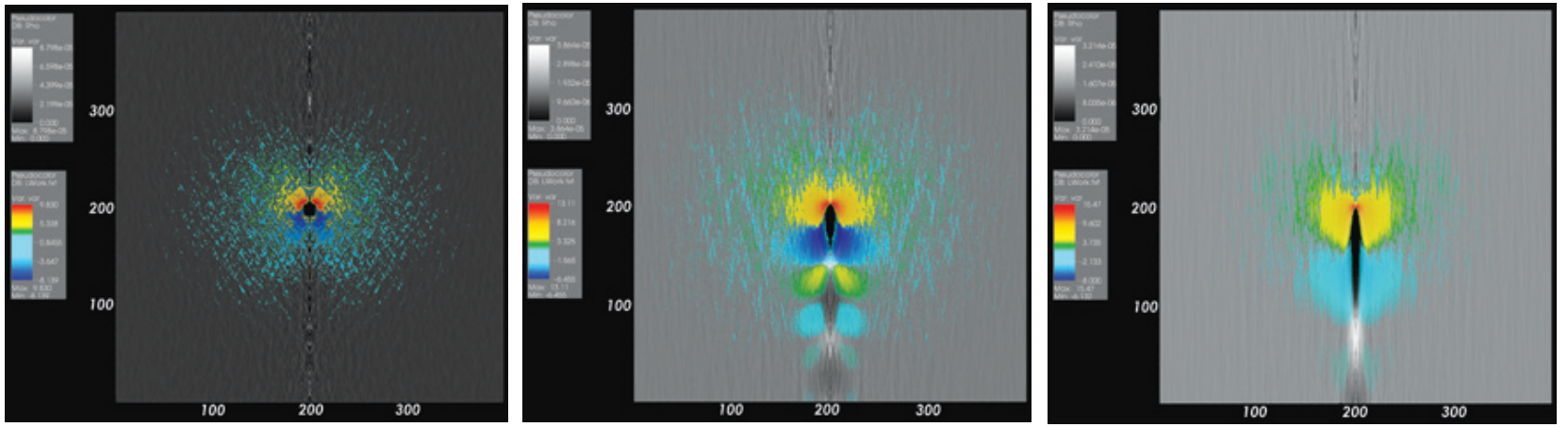

Fig. 1. The wake field is shown for a Z=-2 projectile near the center of the image, moving in the positive y direction. The field of view is 720 Å, compared to the cell length of 1075 Å; the screening length is 2.4 Å. The electron charge density, ρ, is shown in gray; the strongly-repulsive screening cloud is the dark lozenge. The logarithm of the energy transfer field, ϕ, is shown in color. (Specifically, Sign(ϕ) ln(Abs(ϕ)) is shown with a cutoff at small values.) All results are time-averaged over the 400 fs duration of the simulations and are cylindrically-averaged around the axis of the particle trajectory.

Figure 1 (a–c) shows the electron density, ρ, around the moving projectile, and a color image of the energy deposition field, ϕ, is superposed as well. Both fields are time averages of the instantaneous particle distributions. The energy transfer field is $\phi(r)f(r)\cdot(-\nabla V_{coul}(r))$ in terms of the Coulomb potential of the projectile taken at the origin. This is the differential work performed on the target electrons by the projectile; the total rate of projectile energy loss is $dE/dt=\int\phi(r)d^3r$. In the future, we will generalize this to a two-component plasma in which separate current-density fields of electrons and fuel ions will be used to compute the electron-fuel energy split.

In the figure, we note familiar qualitative features of the wake response. At low velocities, the projectile is surrounded by an approximately isotropic screening cloud and approaches Brownian motion from nearly random collisions with the electrons. Since the projectile's energy is $E > 3kT/2$, there is still a net energy loss $dE/dx>0$ composed of a small positive transfer of energy in front of the projectile and a small negative transfer behind. In the intermediate velocity case $v \sim 9\, v_{th}$, the major part of the energy transfer occurs in front of the projectile via strong particle-particle collisions with the electrons in the target. The dynamic collective response leads to damped plasma oscillations in the tail behind the moving projectile. These are visible in the grayscale density ρ and in the faint alternations in the energy flow from projectile to target. The wavelength in the wake scales with projectile velocity and plasma oscillation period is $\lambda \sim v\tau_\rho$. At high velocities, the energy deposition is very strongly concentrated in front of the moving projectile as the projectile plows into the electrons, which have little time to respond. The screening cloud becomes increasingly elongated and the wavelength of the wake oscillations increases, as expected.

In summary, we have developed a state-of-the-art MD capability for studying the energy-loss charged particles in dense plasmas. The tools that we have developed will be extended to more realistic models of the fuel, which include the ionic fuel itself. Simulations of such plasmas will allow us to address the important issue of energy flow in fast ignition targets, including direct coupling from the projectile to the ionic fuel, and the indirect path that relies on electron-ion collisions. Moreover, we are adding thermonuclear burn processes as well, and we will eventually also track fast alpha particles generated by fusion events.

[1] Tabak, M., et al., *Fusion Sci Tech* **49,** 254 (2006).
[2] Richards, D.F., et al., "Beyond Homogeneous Decomposition: Scaling Long-range forces on Massively Parallel Systems," *Proc Conf High Perform Comput Network Storage Anal,* ACM, NY (2009).

Funding Acknowledgments
LLNL Laboratory Directed Research and Development-SI